Silicon (111) - Aluminum (111) - Amorphous Alumina: Asymmetric Quantum Well and Band Alignment

H. Jin[1] and Alexander A. Demkov[1]
[1]*Department of Physics, The University of Texas at Austin, Austin, Texas 78712, USA.*

Thin single crystal films of Al can be epitaxially grown on Si(111) [1]. When taken out of ultra-high vacuum, Al oxidizes and forms a quantum well structure Si-Al-Al_2O_3. Theoretical calculations can shed light on finding the band alignment across the hetero-structure and its electronic and optical properties. However, one needs to build a structural model. The structure of Al on Si(111) has been experimentally determined via the electron microscopy by McSkimming et al. [1]. The Al layer is found to be (111) oriented, with a linear ratio of 3 Si to 4 Al atoms along the interface. Using this information, we construct a periodic model of Si-Al interface and perform density functional theory (DFT) calculations to find the relaxed structure, layer-projected density of states, and planar averaged potential across the interface. From there, we find the band alignment using the valence band offset from the bulk averaged potential. When aluminum metal is exposed to air, a several nanometers thick layer of alumina rapidly forms [2]. This oxide layer is amorphous. We simulate the structure of amorphous alumina using ab-initio molecular dynamics with the melt-and-quench technique [3]. This amorphous alumina can then be directly combined with the previous system to form an asymmetrical quantum well, where the well states and band alignment can be directly obtained from the DFT calculations.

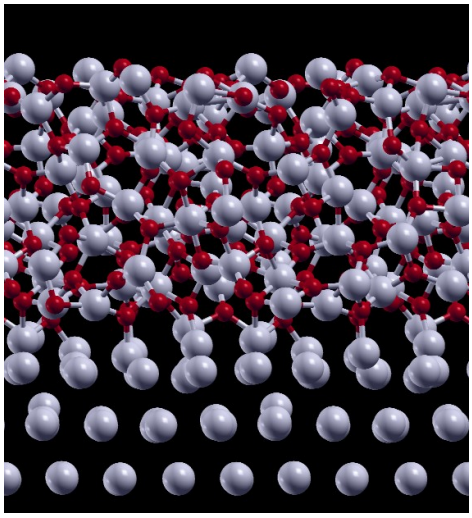

Figure 1. Al-Al_2O_3 interface structure. Red: O; Grey: Al

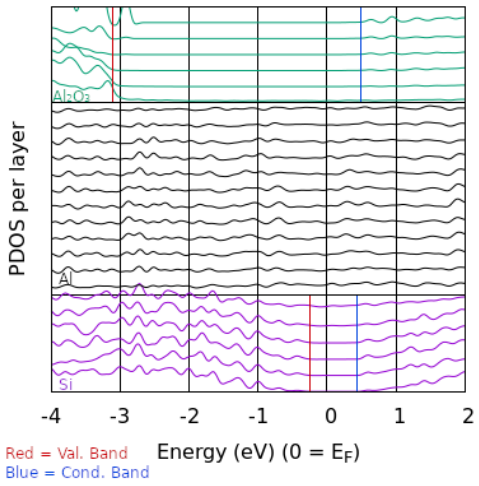

Figure 2. Layer projected DOS of Si-Al-Al_2O_3 asymmetric quantum well.

[1] McSkimming, B. M., Alexander, A., Samuels, M. H., Arey, B., Arslan, I., & Richardson, C. J. (2016). Metamorphic growth of relaxed single crystalline aluminum on silicon (111). J. Vac. Sci. & Technol. A **35**, 021401 (2017).

[2] Jeurgens, L. P., Sloof, W. G., Tichelaar, F. D., & Mittemeijer, E. J. Growth Kinetics and mechanisms of aluminum-oxide films formed by thermal oxidation of aluminum. Journal of Applied Physics, **92**, 1649 (2002).

[3] Gutiérrez, G., asnd Johansson, B. Molecular dynamics study of structural properties of amorphous Al_2O_3. Physical Review B **65**, 104202(2002).